

COMPUTATIONAL APPROACHES TO DETERMINING ISOTHERMAL COMPRESSIBILITY AND FLUCTUATION PARAMETER OF LIQUIDS

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The Fluctuation Theory-based Tait-like Equation of State (FT-EoS) proposed in the work [1], $\rho = \rho_0 + k^{-1} \log [k\rho_0\kappa_T^0(P - P_0) + 1]$, which is shown as a tool for the high accurate prediction of the density under high pressures in liquid matter, varying from organic to ionic liquids [2], require a knowledge not only the density ρ_0 at normal or saturated pressure P_0 but also the isothermal compressibility as its derivative included into the parameter k at the respective conditions.

Here we consider practical spreadsheet-based program implementations of procedures for their computations based either on the reference experimental data, such as the density, the isobaric heat capacity, and the speed of sound, or on the purely predictive methods utilizing the data on molecular structure and parameters and a group contribution approach. The latter set of methods allows also determining the speed of sound in hydrocarbon liquids referring to properties presented in standard databases such as DIPPR 801 (AIChE) [3] discussed in the context of molecular packing and the density fluctuations. In addition, the general algorithm of the usage of parsing SMILES chemical identifier aimed to be used in different group contribution methods for calculating thermodynamic properties will be presented supplied with routines, which do not require a coding on user's end.

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